Least-Squares Deconvolution of Compton Telescope Data With the Positivity Constraint

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ABSTRACT

We describe a Direct Linear Algebraic Deconvolution (DLAD) approach to imaging of data from Compton γ-ray telescopes. Imposition of the additional physical constraint, that all components of the model be non-negative, has been found to have a powerful effect in stabilizing the results, giving spatial resolution at or near the instrumental limit. A companion paper (Dixon *et al. 1993)* presents preliminary images of the Crab Nebula region using data from COMPTEL on the *Compton* Gamma-Ray Observatory.

1. INTRODUCTION

Compton gamma-ray telescopes, despite excellent rejection of the instrumental background, have been handicapped by complicated imaging properties. Conversion of data from such instruments into images is a special case of the linear inverse problem, which occurs again and again in astrophysics (e.g., Craig and Brown, 1986). Linear methods such as linear least-squares (LLSQ) have not generally been effective for Poisson deconvolution problems, despite their dominance in model-fitting. Rather Poisson deconvolution has mostly fallen to such nonlinear approaches as the maximum likelihood and maximum entropy methods.

Nevertheless, linear methods have many advantages that could make them attractive were their defects overcome. Here we describe a linear approach to the inversion of data from Compton telescopes that avoids some of the problems previously encountered. The requirement that all sources be non-negative has a crucial effect, stabilizing the method against ill-conditioning.

2. LEAST-SQUARES DECONVOLUTION OF POISSON DATA

Four parameters characterize each event from an ideal Compton γ-ray telescope: total energy (E), scattering angle (θ), and the celestial co-ordinates (α, δ) of the vector connecting the two interaction points. We bin the data space $\mathcal{I}$ into $I = I_E \times I_\theta \times I_\alpha \times I_\delta$ total bins, where E is binned by $i_E = 1, \ldots, I_E$, θ by i_θ, *etc.* Given J sources, we write for each data bin that the expectation of the counts n_i is a sum with a term for each source:

$$\bar{n}_i = \sum_{j=1}^{J} A_{ij} F_j \,, \tag{1}$$

where the data bins have been ordered by the single index $i = 1, \ldots, I$ combining $(i_E, i_\theta, i_\alpha, i_\delta)$. The elements A_{ij} of the $I \times J$ matrix A (called the *design matrix*), are constants, known if the source positions and instrument response function are given. The F_j are the unknown fluxes of the sources.

Equation (1) has the form of a linear transformation of the space $\mathcal{J}$ of source fluxes into the data space $\mathcal{I}$. This linearity results from the fact that γ-ray telescopes are essentially linear instruments; i.e., the response due to a sum of sources is equal to the sum of the responses taken separately[1] Note that equation (1) can be generalized

[1] At this point in the argument we take the point of view that negative data and model vectors are mathematically sensible, but do not occur physically. This is required for the model and data spaces to be linear vector spaces. The requirement of positivity is considered in Section 3 *ff*.

to take account of linear models for the instrument background simply by inclusion of appropriate extra terms. We assume herein that such terms have been added as needed.

In the model-fitting situation we solve equation (1) with a LLSQ algorithm (e.g., Eadie *et al.* 1971; Press *et al.* 1986) to obtain estimates $\hat{F}_j$ of the fluxes F_j:

$$\hat{F}_j = \sum_i \mathcal{A}_{ij} n_i, \tag{2}$$

where $\mathcal{A}_{ij}$ are functions of the A_{ij}. But for deconvolution do not know the source positions, and hence can no longer calculate the A_{ij} *a priori.*

Therefore we enlarge the model space by covering it with a grid of sources (pixels) at known positions. If the pixels were placed at all possible positions *('distinguishable by the instrument)*, the problem would be formally the same as for equation (1), to be solved by LLSQ. We would expect to obtain a result statistically consistent with zero for pixels with no source, and the correct fluxes for those at the positions of real sources.

Unfortunately this approach has usually failed completely in practice, either duc to singularity of the normal matrix ($A^T A$), or to resulting images which contain noise that overwhelms the expected signal. Strong anticorrelation among adjacent pixels causes oscillations between large positive and negative fluxes. These problems arc due to at least three distinct causes: First, since the number of data bins is typically very large, the number of counts per bin is usually small. Many algorithms (e.g., Bevington 1969, REGRES with MODE$=-1$) for fitting Poisson data by linear least-squares (PLLSQ algorithms) do not work reliably for small numbers of counts per bin. Second, spacing the model grid closer than the intrinsic instrument resolution leads to nearly singular normal matrices, with very large elements in the inverse normal matrix, and oscillatory behavior. Finally, because the number of terms in the mode] is typically large, computational problems may arise in simpler matrix algorithms. Near-singularity due to too fine a grid exacerbates precision difficulties arising from the size of the design matrix.

Each of these maladies infecting PLLSQ deconvolution is effectively curable: First, a method of multi-parameter LLSQ fitting to Poisson data which works in the limit of small numbers of counts has been developed for high-resolution γ-ray spectroscopy and other purposes (Wheaton *et al. 1993).* It is shown therein that weighted LLSQ is unbiased for arbitrarily small counts if the normalized weights (w_i, where $\sum_i w_i = 1$) for each equation i and the count data n_i arc independent. Note that the commonly used approximation $w_i = 1/\sigma_i^2 \approx 1/n_i$ violates this condition and must be avoided. Second, care in choosing the spacing of the model grid can control the second problem. The condition of the design matrix is typically extremely sensitive to too fine a choice of binning in the model space. Finally, Singular Value Decomposition (SVD; see, e.g., Press *et al.* 1986) is essential in practice because it allows even very large, singular or nearly singular systems to be solved on subspaces which are unaffected by any linear dependences among the columns of A, without serious numerical precision problems.

These methods together have made Direct Linear Algebraic Deconvolution (DLAD) practical in many situations where it has previously been ineffective. Based on our experience with it, the main problem is in determining the finest pixel spacing that can be used, This latter obstacle has been effectively removed by a taking advantage of onc further essentially physical fact, of which linear algebra knows nothing: all real sources must be non-negative. This constraint dramatically improves the attainable resolution.

3. THE POSITIVITY CONSTRAINT

There are reasons to expect the positivity constraint to be especially important for dcconvolution. First, as noted above, when the pixels arc too finely spaced, the result is a strong anti-correlation between adjacent image elements, and resulting oscillatory behavior. Positivity forces the negative excursions in the image to rise to zero, and it also forces adjacent positive excursions to decrease correspondingly, because of the anti-correlation. The result is to flatten the images, strongly suppressing features not statistically required.

A heuristic argument illustrates another aspect of the power of the positivity constraint for recovering astronomical images, where most pixels are zero, from data equations like Eqn. (1), Consider a simple image consisting of a 3 x 3 field of 9 pixels. Given, e.g., row and column sums, we would have six equations of the form (l), but with J = 9, no solution would be possible. If several row and column sums were zero it would not help because of the possibility of canceling negative and positive pixels. But using positivity, a row or column sum of O would imply *all three* of the corresponding pixels were also zero: that is it would be equivalent to *three* additional equations, not one. Thus not only does the constraint suppress noise, in effect it may also bring in many further equations, so that undcrdctcrmined singular systems become tractable.

Equation (2) yields an identity if applied to the *expected* counts $\bar{n}_i$ and substituted into equation (1), when it must yield a positive solution for a positive model. If then we could repeat the experiment many times to obtain ncw data sets like $(n_1, \ldots n_I)$, the ensemble of their corresponding estimates would be distributed so that the iso-probability surfaces, $\approx$ inclined J-dimensional ellipsoids, would bc centered on the true solution, $(F_1, \ldots F_J)$. If the tots] expected counts $(\sum_i \bar{n}_i)$ >> 1, the distribution is virtually normal. Because of the finite extent of the probability ellipsoid, the solution for any single *observed* data set $\{n_i\}$ can be outside of the positive region.

For a single gaussian trial, the likelihood function (e.g., Eadie *et al.* 1971) for the true answers would be peaked in an ellipsoid, similar to the onc dcscribcd above, but centered at the point estimate, equation (2). The positivity constraint excludes values outside the first quadrant[2], so we set the likelihood zero elsewhere. There results a truncated multi-normal distribution, with a maximum on the boundary of the first quadrant if the point estimate (2) is outside it; as it is, almost always, in deconvolution problems. Inside or outside, wc take the co-ordinates of the maximum to be the best solution.

4. EXPERIENCE WITH SUBROUTINE NNLS

While working toward an algorithm to find the above maximum, we discovered a pre-existing subroutine which dots much of what wc need. The FORTRAN subroutine NNLS (Lawson and 11 anson 1974), given an I x J design matrix A and]-vector $\vec{b}$, solves the overdetermined system

$$\vec{\mathbf{b}} = \mathbf{A}\vec{\mathbf{x}} \tag{3}$$

for $\vec{x}$ in least-squares, subject to the constraint that $x_j \geq 0$.

It has been possible to usc much fmcr pixel grids with NNLS than previously. images of the Crab Nebula region with COMPTEL (Dixon *et al.* 1993) show that the spatial resolution obtained is essentially the instrumental resolution. Sources not centered on a pixel yield adjacent peaks, the centroid of their flux corresponding closely to the true source position, If the pixel grid is refined too far, the image of a source breaks up into a cluster of adjacent peaks, whose total flux is essentially that of the single source peak seen at lower resol ut ion.

For data of very high statistical quality, all pixels in the image arc positive without constraint. But on re-analyzing the data with a finer pixel grid, the oscillations will appear, and positivity can bc invoked to stabilize the result. Thus for high-statistics data, the effect of positivity is to allow the effective resolution to be pressed beyond what would otherwise bc possible.

A problem not yet solved is the combination of partial data sets. In a series of simple source-background subtractions (i. e., J = 2 fits), when the net source estimates are not significant so that many arc negative, it is of course a serious error to discard the negative estimates (or set them to zero) and average the remainder. Such a procedure

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[2] **Where no confusion can arise, we call the 2^J regions of uniform signature, such as (+ + + . ..+ ++), "quadrants" even for $J > 2$.**

would introduce a large bias. In general, simple averages of constrained results are biased. We are currently pursuing a. method of combination based on multiplication of the multi-normal functions for each data set.

5. PROBLEM AREAS AND EXTENSIONS

'The NNLS routine described in the previous section has allowed the effect of the positivity constraint to be explored in a useful preliminary way. However several problems remain which prevent the current method from giving a wholly satisfactory solution to the practical problems in real data analysis: First, NN 1,S gives no direct information concerning the uncertainties in the answers and requires a complete matrix solution for each data set, as nothing like an inverse matrix is available. Also, while based on the experience we have had in solving large COMPTEL problems the practical advantages of SVD are mostly preserved in NNLS, the SVD matrix factors (U, W, and V, Press *et al.* 1986) are not directly returned. In the current form of the algorithm, the large model space $\mathcal{J}$ and data space $\mathcal{I}$ imply that very large matrices must be manipulated. For the present, this requires a supercomputer. Finally, there are still theoretical questions, especially concerning the combination of results for partial data sets.

We believe we understand how to remedy all these problems in principle. Ideas for an algorithm, which would run after SVD and yield the best constrained LLSQ solution, are currently being tested. There are also several ways in which the size of the matrices which have to be manipulated can eventually be reduced, probably by two orders of magnitude or more.

6. CONCLUSION

Based on theoretical considerations, verified by studies with Monte Carlo data, calibration and balloon data with the UC Riverside γ-ray telescope, and flight data from the CO MPTEL experiment on *CGRO*, we conclude as follows: First, DLAD is a useful complement to more traditional non-linear approaches if care is taken to observe the precautions set forth in Section 2. Second, limitations on the resolution can be very markedly relaxed by taking advantage of one additional *physical* constraint, that all real sources are non-negative. While considerable work remains to fully implement DLAD with the positivity constraint, use of the NNLS subroutine of Lawson and Ran son (1974) has allowed its power to be verified and explored. The results to date (Dixon *et al.* 1993) have been very encouraging.

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